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% Male Rat Lung In Vitro MCMC simulation file
% Three chains can be run by selecting different seernd
% and changing the output file name
prepare @all
output @clear

VVIALF=0.01165; %% Male ==VVIAL=.0119573;
VVIALM=0.0119573;
VMED=.001;
VINJF=0.0002; %% Male ==VIN=0.0003858 !important
VINM=0.0003858 ;
VAIRF=VVIALF-VMED;
VAIRM=VVIALM-VMED;
TSTOP=1.2;
TF=0.;
TI=0.2;
PROT = 1.0;
P1 = 0.69;
WESITG=0;
WEDITG =0;

CINT = 0.1 ;
MAXT = 0.01 ;
TSTOP = 1.1 ;
KG1 = 0.45 ;

seedrnd(45526)
%seedrnd(334485)
%seedrnd(998754)

global _cal
global _time
global data
global tFindex
global tMindex

global CCC
global firstT
global lastT
global firstD
global lastD
global ControlData

use ControlData.m
use FemaleData.m
use MaleData.m

dataF = [FratFLung(:,IDf_270ppm : IDf_50ppm) ];
dataM = [FratMLung(:,IDm_529ppm : IDm_264ppm) ];

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data = NaN* ones([10, 5]); % corresponse to max 25 timepoints and 5 dose
each gender
data(1:6, 1:3) = dataF ;
data(1:10, 4:5) = dataM;
firstT = [1, 1]
lastT = [6, 10]
firstD = [1, 4]
lastD = [3, 5]
tFindex = FratFLung(:, IDf_time);
tMindex = FratMLung(:, IDm_time);

AA=dataF(1,:) * (VAIRF+P1*VMED);
BB=dataM(1,:) * (VAIRM+P1*VMED);
CCC = [AA, BB];
data = log(data);

function preds = getpreds(Vk, A10, Gender)
    global _cal
    global _time
    global tFindex
    global tMindex
    global ControlData

    % draw back ground loss rate
    tmp = ceil(rand*500);
    lossR = ControlData(tmp);

    setmdl("VK", exp(Vk));
    setmdl("A10", A10);
    setmdl("RLOSS", exp(lossR));

    if Gender==1
        tindex = tFindex;
        setmdl("VVIAL", 0.01165);
        setmdl("VINJ", 0.0002);
    else
        tindex = tMindex;
        setmdl("VVIAL", 0.0119573);
        setmdl("VINJ", 0.0003858);
    end

    data @clear
    data("SAMPTIMES", ["T"], tindex);

    start @nocallback

    preds = NaN*ones(length(tindex), 1);

    for i = 1:length(tindex)
        idx = find(_time == tindex(i));
        if(idx ~= [])
            preds(i) = max(0.0, _cal(idx));
        end
    end
end

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```
preds = log(preds);  
end  
  
use ".\MCMCscripts\invitromc12mrl.m"  
  
chains = runmcmc();  
  
save @file=mratlungred01.dat @format=ascii @separator=tab chains
```